

Coulomb deexcitation of pionic hydrogen within close-coupling method

V. N. Pomerantsev, V. P. Popov
Institute of Nuclear Physics, Moscow State University

The Coulomb deexcitation of (πp) atom in collisions with the hydrogen atom has been studied in the fully quantum mechanical close-coupling approach for the first time. The total Coulomb deexcitation cross-sections of $nl \rightarrow n'l'$ transitions and l -averaged cross-sections are calculated for $n = 3 - 8$ and at the relative energies $E = 0.01 - 100$ eV. The strong interaction and vacuum polarization shifts of ns -states are taken into account. It is shown that the $\Delta n > 1$ transitions are very important and make up a substantial fraction of the Coulomb deexcitation cross-section (up to $\sim 47\%$).

Exotic hydrogen atoms are formed in highly excited states and the evolution of their distributions on the quantum numbers and kinetic energy is defined by the competition of both collisional and radiative deexcitation processes during the atomic cascade. The interest in the problem attracted special attention after the experimental observation of a high energy fraction ($\gg 1$ eV) in the energy distribution of the pionic atoms at the instant of the charge exchange reaction $\pi^- p \rightarrow \pi^0 n$ was obtained [1, 2, 3, 4]. The observed Doppler broadening of the neutron time-of-flight (NTOF) spectra in the experiments are attributed to the Coulomb deexcitation (CD) process, where the energy of the transition is shared between the colliding objects. In order to analyze the above mentioned and the new experiments [5, 6, 7, 8] on the precision spectroscopy of K X -rays from pionic atoms, the kinetic-energy distribution of pionic hydrogen must be calculated from a realistic cascade model.

The first theoretical study has been carried out in the framework of the two-state semiclassical model [9] with some additional approximations (e.g., $n \gg 3$). Later, the process was considered within the advanced adiabatic [10] (see also references therein), and the classical-trajectory Monte Carlo [11] approaches. While for the low n states the approaches [9, 11] cannot be expected to give a reliable description of the CD process, the CD cross sections obtained in [10] for the $n \rightarrow n-1$ transitions ($n = 3-5$) are smaller about one order of the magnitude than in [9] and too small to explain the experimental data [12]. Therefore, in the most important region of $n = 3-7$ relevant for the atomic cascade the theoretical results are rather undefined and this process is regarded as the least known process of the pionic cascade.

In this paper, we report the results for the CD process of $\pi^- p$ atom in collisions with H obtained for the first time in the framework of the fully quantum mechanical approach. We use the close coupling (CC) method, in which the scattering processes

$$(\pi^- p)_{nl} + H_{1s} \rightarrow (\pi^- p)_{n'l'} + H_{1s}, \quad (1)$$

such as elastic scattering ($n' = n, l' = l$), Stark transitions ($n' = n, l' \neq l$), and CD ($n' < n$) are described in unified manner. The method has been recently employed for the study of the CD process in muonic hydrogen [13], where substantially new results in comparison with the known in the literature [9, 14] (see references therein) have been obtained. Unless otherwise stated the atomic units ($\hbar = e = m_e m_p / (m_e + m_p) = 1$) will be used throughout the paper.

The Hamiltonian of the system $((\pi^- p)_{nl} + H_{1s})$ (after separation of the c.m. motion) is given by

$$H = -\frac{1}{2m} \Delta_{\mathbf{R}} + h_{ex}(\boldsymbol{\rho}) + h_H(\mathbf{r}) + V(\mathbf{r}, \boldsymbol{\rho}, \mathbf{R}), \quad (2)$$

where m is the reduced mass of the system, \mathbf{R} is the radius vector between the c.m. of the colliding atoms, $\boldsymbol{\rho}$ and \mathbf{r} are their inner coordinates. The interaction potential, $V(\mathbf{r}, \boldsymbol{\rho}, \mathbf{R})$, is a sum of four Coulomb pair interactions between the projectile atom and the target atom particles. $h_{ex}(\boldsymbol{\rho})$ and $h_H(\mathbf{r})$ are the hydrogen-like Hamiltonians of the free exotic and hydrogen atom, whose eigenfunctions together with the angular wave function $Y_{LA}(\hat{\mathbf{R}})$ of the relative motion form the basis states, $|1s, nl, L : JM\rangle$, with the conserving total angular momentum (JM) and parity $\pi = (-1)^{l+L}$. The total wave function of the system can be expanded as follows

$$\Psi_E^{JM\pi}(\mathbf{r}, \boldsymbol{\rho}, \mathbf{R}) = R^{-1} \sum_{nlL} G_{nlL}^{J\pi}(R) |1s, nl, L : JM\rangle. \quad (3)$$

The expansion (3) leads to the close-coupling second order differential equations for the radial functions of the relative motion, $G_{nlL}^{J\pi}(R)$,

$$\begin{aligned} \left(\frac{d^2}{dR^2} + k_n^2 - \frac{L(L+1)}{R^2} \right) G_{nlL}^{J\pi}(R) = \\ = 2m \sum_{n'l'L'} W_{n'l'L',nlL}^{J\pi}(R) G_{n'l'L'}^{J\pi}(R). \end{aligned} \quad (4)$$

The channel wave number is defined as $k_n^2 = 2m(E_{cm} + E_{n_0 l_0} - E_{nl})$, where E_{cm} and $(n_0 l_0)$ are the energy of the relative motion and the exotic atom quantum numbers in the entrance channel, respectively. The bound energy of πp atom, $E_{nl} = \varepsilon_{nl} + \Delta\varepsilon_{nl}$, includes the eigenvalue of $h_{ex}(\boldsymbol{\rho})$, ε_{nl} , and the energy shift, $\Delta\varepsilon_{nl} = \Delta\varepsilon_{nl}^{vp} + \Delta\varepsilon_{nl}^{str}$, due to the vacuum polarization and strong interaction. Hereafter, the energy E_{cm} will be referred to $\varepsilon_{nl \neq 0}$ in the entrance channel (we assume that $\Delta\varepsilon_{nl \neq 0} = 0$)¹.

The matrix elements of the interaction potential,

$$W_{n'l'L',nlL}^{J\pi}(R) = \langle 1s, n'l', L' : JM | V | 1s, nl, L : JM \rangle \quad (5)$$

¹ The strong interaction shifts are calculated according to $\Delta\varepsilon_{ns}^{str} = \Delta\varepsilon_{1s}^{str}/n^3$, where $\Delta\varepsilon_{1s} = -7.11$ eV from [15]). The next values [16] (-3.24 eV (1s), -0.37 eV (2s), and -0.11 eV (3s)) for the vacuum polarization shifts are used in the calculations. For $n > 3$ we assume $\Delta\varepsilon_{ns}^{vp} = \Delta\varepsilon_{n-1,s}^{vp}((n-1)/n)^3$.

are obtained by averaging it over the electron wave function of the $1s$ -state and then applying the multipole expansion. The integration over $(\boldsymbol{\rho}, \hat{\mathbf{R}})$ reduces the matrix elements (5) to the multiple finite sum.

At fixed E_{cm} the coupled differential equations (4) for the given J and π values are solved numerically by Numerov method with the standing-wave boundary conditions involving the real symmetrical K -matrix related to T -matrix by the equation $T = 2K/(I - iK)$. All exotic atom states with n values from 1 up to n_0 have been included in the close-coupling calculations. The following cross sections will be discussed:

- partial cross section

$$\sigma_{nl \rightarrow n'l'}^J(E) = \frac{\pi}{k_n^2} \frac{2J+1}{2l+1} \sum_{LL'\pi} |T_{nlL \rightarrow n'l'L'}^{J\pi}|^2, \quad (6)$$

- total cross section of the transition $nl \rightarrow n'l'$

$$\sigma_{nl \rightarrow n'l'}(E) = \sum_J \sigma_{nl \rightarrow n'l'}^J(E), \quad (7)$$

- total cross section from ns - state

$$\sigma_{ns \rightarrow n'}(E) = \sum_{l'} \sigma_{ns \rightarrow n'l'}(E), \quad (8)$$

and the l -averaged cross section ($l > 0$)

$$\sigma_{nn'}^{l>0}(E) = \frac{1}{n^2 - 1} \sum_{l>0, l'} (2l+1) \sigma_{nl \rightarrow n'l'}(E). \quad (9)$$

We assume the pionic atom states with $l \neq 0$ are degenerated and so the l -averaged cross section (9) can be used to illustrate the basic features of the CD process.

The CC calculations of the CD cross sections Eqs. (6-9) were carried out for $(\pi^- p)_{nl} + H$ collisions for $n = 3-8$ and at energy range $E_{cm} = (0.01 - 100)$ eV. Summation over the partial waves in Eq. (6) was done up to a value J_{max} until an accuracy better than 0.1% was reached at all energies. The analysis of the J dependence of the partial cross sections $\sigma_{nl \rightarrow n'l'}^J$ shows that most the CD cross sections give the partial waves with rather low J values as compared with the elastic scattering and Stark transition processes. Besides, our study shows that a significant underestimation of the CD cross sections (up to one order of the magnitude) can be obtained if one neglects the higher multipole terms in the expansion of the coupling matrix (5). Such a strong effect together with the relatively low J values involved in the inelastic transitions are related with the fact that the CD process is determined by the comparably more short-range interaction.

In order to illustrate the influence of the ns state energy shifts on the CD cross sections, the calculations were performed both with and without taking energy shifts into account. The effect is the most pronounced for the low-lying states and some of the results for $n = 3, 4$ are shown in Figs. 1, 2 and presented in Table I.

The CD cross sections for a number of transitions $3l \rightarrow 2l'$ with or without the energy shifts of the ns -states are shown in Fig. 1. In the case $\Delta\varepsilon_{ns} \neq 0$ the energy dependence of the cross sections changes crucially. The

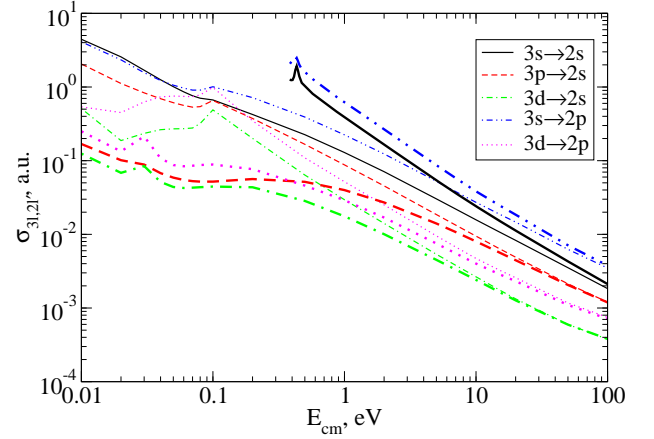


FIG. 1: The CD cross sections $\sigma_{3l,2l'}$ for $(\pi p)_{3l} + H$ collisions calculated both with (thick lines) and without (thin lines) taking the ns -state energy shifts into account.

cross sections corresponding to the $3p(3d) \rightarrow 2s, 2p$ transitions at energies above and below the threshold of the Stark transitions $3s \rightarrow 3p, 3d$ are strongly suppressed. The effect is more clearly observed at energies in the vicinity of 0.1 eV (the suppression is more or about one order of the magnitude). At $E_{cm} \gg |\Delta\varepsilon_{ns}|$ the differences between the corresponding pair of the curves (see Fig. 1) are negligible at $E_{cm} \geq 15$ eV for $n = 3$ and at $E_{cm} \geq 1$ eV for $n = 4$. On the contrary, the transitions $3s \rightarrow 2s, 2p$ are enhanced at the threshold by a factor about 3 – 4. The main reason of such behavior of the CD cross section is related with the inelastic nature of the Stark transitions between the splitted upper states.

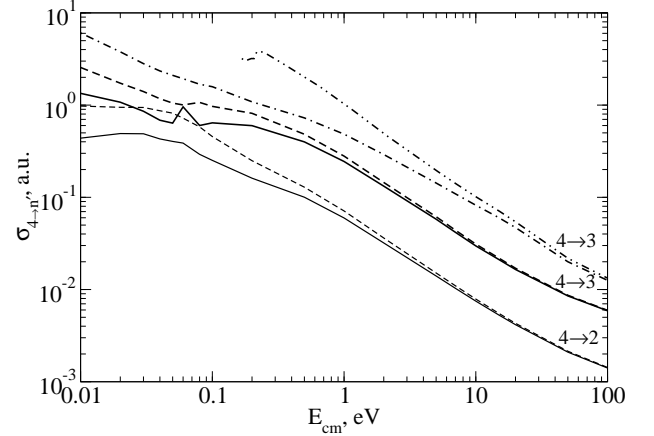


FIG. 2: The l -averaged CD cross sections $\sigma_{4,3}^{l>0}$ (thick lines) and $\sigma_{4,2}^{l>0}$ (thin lines) for $(\pi p)_4 + H$ collisions calculated with (solid lines) and without (dashed lines) taking the s -states energy shifts into account. The CD cross sections $\sigma_{4s \rightarrow 3}$ calculated both with (double-dot-dashed line) and without (dot-dashed line) taking the s -state energy shifts into account are also shown.

The similar regularities are also observed in the l -averaged CD cross sections. In Fig. 2 (see also Table 1) the l -averaged CD cross sections for the $4 \rightarrow 3$ and $4 \rightarrow 2$ transitions and total cross sections from $4s$ -state are presented. One can see that the maximal suppression due to

TABLE I: The CD cross sections $\sigma_{n,n'}^{l>0}$ for $(\pi p)_n + H$ collisions calculated in quantum-mechanical CC approach.

$E_{cm}, \text{ eV}$	0.01	0.02	0.03	0.05	0.08	0.1	0.2	0.5	1.0	2.0	5.0	7.0	10	20	50	100
σ_{32}	0.409	0.231	0.289	0.145	0.138	0.143	0.139	0.102	0.072	0.046	0.022	0.017	0.012	0.007	0.003	0.002
$\sigma_{32}^{(\Delta=0)}$	2.261	1.315	1.293	1.303	1.275	1.711	0.770	0.293	0.148	0.075	0.030	0.021	0.015	0.008	0.004	0.002
σ_{43}	1.342	1.076	0.858	0.638	0.958	0.642	0.599	0.399	0.245	0.132	0.058	0.042	0.030	0.017	0.009	0.006
$\sigma_{43}^{(\Delta=0)}$	2.558	1.728	1.402	1.052	1.004	0.969	0.814	0.483	0.280	0.145	0.062	0.044	0.031	0.017	0.009	0.006
σ_{42}	0.438	0.491	0.489	0.404	0.387	0.252	0.161	0.100	0.060	0.032	0.014	0.010	0.007	0.004	0.002	0.001
$\sigma_{42}^{(\Delta=0)}$	0.977	0.946	0.942	0.817	0.721	0.456	0.250	0.129	0.071	0.036	0.015	0.011	0.008	0.004	0.002	0.001
σ_{54}	3.497	2.672	1.750	1.201	1.055	0.769	0.531	0.314	0.202	0.125	0.060	0.044	0.033	0.020	0.013	0.012
σ_{53}	0.929	1.118	0.677	0.417	0.355	0.251	0.177	0.091	0.050	0.025	0.010	0.007	0.005	0.003	0.002	0.001
σ_{52}	0.188	0.292	0.199	0.122	0.103	0.074	0.069	0.040	0.022	0.011	0.005	0.004	0.003	0.001	0.001	0.001
σ_{65}	3.644	2.510	2.423	1.544	1.121	1.012	0.636	0.298	0.169	0.098	0.041	0.031	0.024	0.016	0.015	0.020
σ_{64}	1.446	1.309	1.232	0.903	0.683	0.603	0.377	0.217	0.129	0.068	0.028	0.021	0.015	0.009	0.005	0.004
σ_{63}	0.436	0.349	0.265	0.171	0.115	0.098	0.065	0.032	0.017	0.008	0.003	0.002	0.002	0.001	0.001	0.001
σ_{76}	5.647	4.321	3.202	2.636	2.157	1.747	1.247	0.590	0.346	0.190	0.082	0.061	0.045	0.027	0.023	0.038
σ_{75}	1.545	1.272	0.793	0.696	0.762	0.527	0.319	0.150	0.095	0.053	0.023	0.018	0.014	0.009	0.007	0.008
σ_{74}	0.300	0.280	0.154	0.156	0.162	0.114	0.069	0.037	0.019	0.010	0.004	0.003	0.002	0.002	0.001	0.002
σ_{87}	7.480	4.541	4.095	3.379	3.217	2.379	1.757	1.003	0.662	0.371	0.159	0.118	0.086	0.051	0.042	0.077
σ_{86}	1.340	0.925	0.822	0.719	0.624	0.485	0.378	0.190	0.130	0.072	0.031	0.023	0.017	0.011	0.010	0.016
σ_{85}	0.571	0.340	0.315	0.362	0.234	0.222	0.170	0.078	0.044	0.023	0.010	0.008	0.006	0.004	0.003	0.004

the energy shift of $4s$ state is weaker and less or about two times at very low energy both for $4 \rightarrow 3$ and $4 \rightarrow 2$ transitions, while at $E_{cm} > 1$ eV does not exceed 15%. The important observation follows from Fig. 2: the CD cross sections for the $\Delta n = 2$ transition are strongly enhanced, in contrast to the calculations [9, 10], and their relative contribution to the total CD transitions $4 \rightarrow n' \leq 3$ varies from 20% up to 39%.

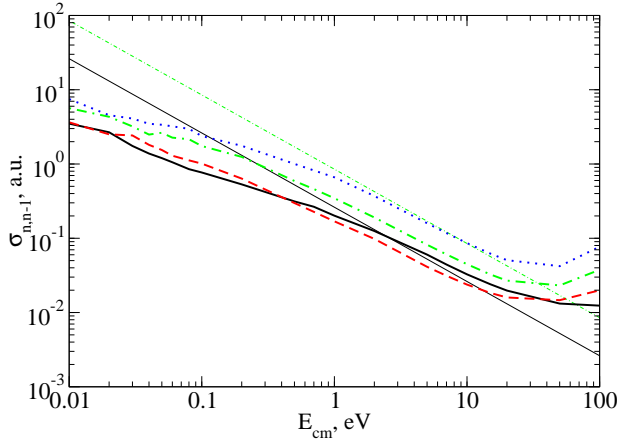


FIG. 3: The l -averaged CD cross sections $\sigma_{n,n-1}^{l>0}$ for $(\pi p)_n + H$ collisions with $n = 5$ (solid line), 6 (dashed), 7 (dot-dashed) and 8 (dotted). The results of the parameterization [11] for $n = 5$ and 7 (thin lines).

Beginning from the paper [9], it is commonly believed that the CD cross sections for $\Delta n = 1$ transitions behave like $\sim n^\gamma / E_{cm}$. The n and E_{cm} dependences of the l -averaged CD cross sections ($l > 0$) for $n = 5 - 8$ are shown in Fig. 3 for the $\Delta n = 1$ transitions. The straight lines show the results of the parameterization [11], based

on the CD cross sections [9] for $n \leq 7$. As it is seen from Fig. 3, the energy dependence of the CD cross sections only in the region $1 \lesssim E \lesssim 10$ eV, as a whole, is in a qualitative agreement with the one like $1/E_{cm}$. But at the energies beyond this interval the CC results don't confirm the $1/E$ energy dependence of the cross sections. In particular, at $E \lesssim 1$ eV and $n > 4$ our results show weaker and rather $1/\sqrt{E}$ behavior of the CD cross sections.

Concerning the power n -dependence nearly to n^γ with $\gamma > 2$, the present consideration doesn't confirm that the CD cross sections have such a scale factor depending on n (see Fig. 3 and Table 1). Moreover, for $n = 4 \div 6$ the non-monotone behaviour of the σ_n^{CD} as a function of n is revealed.

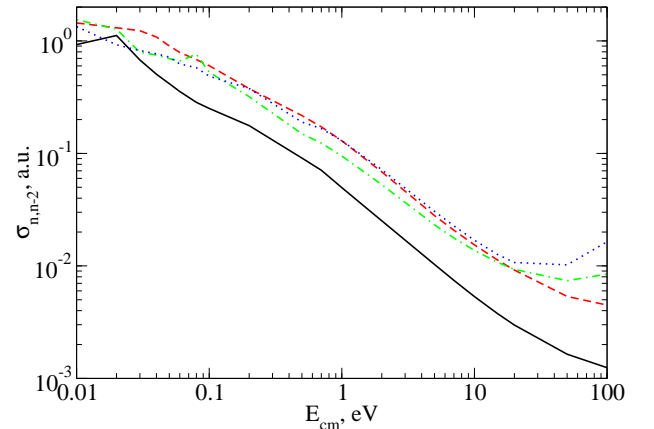


FIG. 4: The same as in Fig. 3 but for transitions $n \rightarrow n-2$.

The present calculations show that $\Delta n = 1$ transitions dominate. According to our CC calculations (see Fig. 4

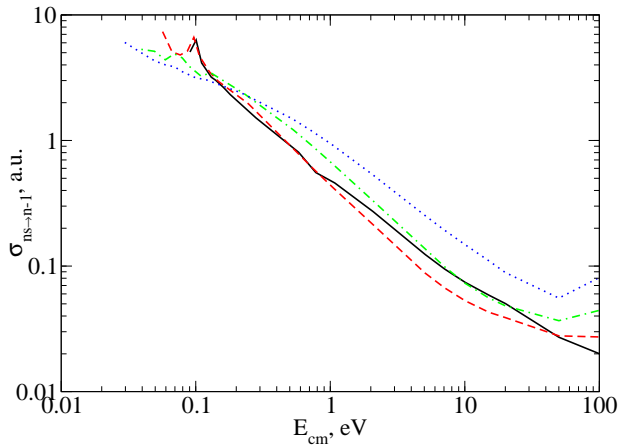


FIG. 5: The CD cross sections from s -states $\sigma_{ns \rightarrow n-1}$ for $n = 5 - 8$. The notations of curves are the same as in Figs. 3 and 4.

² We thank Dr. T. Jensen for the preliminary results of the analysis with the present CD cross sections of the NTOF spectra [3]. Our results explain the high energy component around 105 eV

and Table I), the $\Delta n > 1$ transitions make up a substantial fraction of the total CD cross sections (20–47 %) for $n \geq 4$ at all the energies under consideration. It is worthwhile noting, that there is no simple n dependence of the CD cross sections for the $\Delta n > 1$ transitions. The regular n dependence appears only at the relative energies more or about 50–70 eV.

In summary, the CD process in pionic hydrogen has been studied for the first time in the fully quantum mechanical CC approach, involving simultaneously the elastic and Stark processes. The obtained results reveal the new knowledge about the CD process and are very important for the reliable analysis of the K X-ray yields and NTOF spectra.²

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due to the $5 \rightarrow 3$ transition and lead to a very good agreement with the experimental weight of the $3 \rightarrow 2$ component at 209 eV.

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